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Applied to Multiple Quadratures
and Multiple Scattering**

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A Comparative Study of Conroy and Monte Carlo Methods Applied to Multiple Quadratures and Multiple Scattering

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SUMMARY

This paper discusses an efficient numerical method of multiple quadratures, referred to here as the Conroy method, as applied to the problem of computing multiple scattering contributions in the radiative transfer through realistic planetary atmospheres, and presents a brief error analysis of the method. In these discussions, comparisons are drawn with the more familiar Monte Carlo method. Both methods are stochastic problem-solving models of a physical or mathematical process and utilize the sampling scheme for points distributed over a definite region. However, whereas in the Monte Carlo scheme the sample points are distributed randomly over the integration region, in the Conroy method, the sample points (N_c , in number) are distributed systematically, such that the point distribution forms a unique, closed, symmetrical pattern which effectively fills the region of the multidimensional integration. Conroy has shown that for continuous functions with bounded first derivatives, the error ultimately disappears at least as $1/N_c^2$, whereas, in the Monte Carlo method, the error disappears as $1/\sqrt{N}$, where N is the number of trials in the random sampling. The methods are illustrated by two simple examples: One, of multidimensional integration involving two independent variables, and the other, of computing the second order scattering contribution to the sky radiance.

INTRODUCTION

In aerosol remote sounding techniques, which require the inversion of multiply scattered radiation signals, an object of primary concern is the enormous computational costs involved. The solution of the multiple scattering problems often involves numerical computation of multidimensional integrals with several independent variables. Thus, in order to keep the costs of such numerical inversions from becoming prohibitive, it is imperative that multiple scattering computations for realistic atmospheres be performed efficiently and economically.

This paper discusses an efficient numerical method of multiple quadratures, developed by Conroy (ref. 1) in 1967, and referred to here as the Conroy method, as applied to the problem of multiple scattering calculations. The method and its results are compared with those for the more familiar Monte Carlo method (refs. 2-9), which, as it is known today, had its origins in the 1940's.

Both the Conroy and the Monte Carlo methods are stochastic problem-solving models of either a physical or a mathematical process. An illustration for each of these two types of processes will be discussed in a later section. Both of these methods utilize the sampling scheme for points distributed over a definite region. However, in the Conroy scheme, the sample points are distributed systematically over the region

of integration, whereas, in the Monte Carlo method, they are randomly distributed. In addition, the ensemble of points, in the Conroy method (ref. 1), forms a unique, closed, symmetrical pattern which effectively fills the region of the multidimensional integration. To generate such an arrangement of the sample points, the Conroy method employs certain rational constants. A table of such constants, suitably optimized, which will permit integration of functions with up to 12 independent variables, is given in Table III in reference 1, and is reproduced in Table 1 in this paper. The Monte Carlo method employs a random number generating scheme which governs the random distribution of sample points.

In this paper, a brief statistical-analytic treatment of the error characteristics of the two methods is also discussed. For instance, Conroy (ref. 1) has shown that for continuous functions (of many independent variables) with bounded first derivatives, the error ultimately disappears at least as rapidly as $1/N_c^2$, where N_c is the number of sample points used, whereas, in the Monte Carlo method, the error disappears at the rate of $1/\sqrt{N}$, where N is the number of trials in the random sampling process. In addition, for runs of practical length, the error limits with the Conroy systematic sampling scheme are smaller than those with the Monte Carlo random sampling scheme - by a factor ranging from 2 to perhaps 10^4 or more (ref. 1).

The two methods will be applied to two simple cases: (1) A 2-dimensional integration of a simple mathematical function of two variables, as an example of a nonsimulation type mathematical process; and (2) a 2-dimensional integration as it occurs in the physical process of computing the double scattering contributions to circumsolar sky radiance.

It is a pleasure to gratefully acknowledge the stimulating discussions with John N. Shoosmith on the Monte Carlo method and with Gail Box on the computational aspects in connection with this work.

THE CONROY AND MONTE CARLO METHODS

Consider the following simple 2-dimensional integral

$$I_2 = \int_0^1 \int_0^1 F(x_1, x_2) dx_1 dx_2 \quad (1)$$

Conroy Method

According to Conroy (ref. 1), an approximation to the integral in equation (1) is the sum $S_1(N)$ defined as follows:

$$S_1(N) = \frac{2}{M} \sum_{m=1/2}^N \vec{F}(2\{m\vec{\alpha} - \vec{e}\}) \quad (2)$$

where $F(x_1, x_2) = f(|x_1|, |x_2|)$ may be regarded as a periodic function with period two in each of the variables (x_1, x_2) and

$$x_1 = \frac{P_{x_1}}{M}, \text{ and } x_2 = \frac{P_{x_2}}{M} \quad (3)$$

where the P 's are selected odd integers and N is a positive integer, i.e.,

$$M = 2N + 1 \quad (4)$$

and e_{x_1}, e_{x_2} are integers chosen so that each component of the vector within braces falls within the range $(-1/2, 1/2)$. $F(x_1, x_2)$ is an even function about $(x_1 = 0, x_2 = 0)$ and is evaluated at $M/2$ sample points (ref. 1).

Monte Carlo Method

On the other hand, the application of the Monte Carlo method to the evaluation of the multidimensional integral in equation (1) is explained as follows.

Suppose the experimentally estimated probability of winning a simple game of throw of dice gives the area A underneath the curve

$$y = f(x) \quad (5)$$

then we may define A as

$$A = \int_0^1 f(x) dx \quad 0 \leq f(x) \leq 1 \quad (6)$$

This reasoning can be used to generalize the above process to a multidimensional integral (ref. 2). The efficiency of the process does not depend at all upon the detailed microscopic character of the function $f(x)$ but only on a very gross characteristic - the total area, or in the case of a multidimensional integral, the total multidimensional volume. Thus, the simplest and most direct application of the Monte Carlo method is to the evaluation of multidimensional integrals (ref. 2).

Now consider the functional equation $F(x_1, x_2)$ in two independent variables x_1 and x_2 to be integrated over a definite region in which $g(x_1, x_2)$ is the probability density function (PDF) defined such that

$$0 \leq g(x_1, x_2) \leq 1 \quad (7)$$

For every $g(x_1, x_2)$, there exists a point (x_1, x_2) belonging to the integration region such that

$$\iint g(x_1, x_2) dx_1 dx_2 = 1 \quad (8)$$

The expected value $\langle F \rangle$ for the multidimensional integral of the function $F(x_1, x_2)$ can be represented accordingly

$$\iint F(x_1, x_2) g(x_1, x_2) dx_1 dx_2 = \langle F(x_1, x_2) \rangle = \langle F \rangle \quad (9)$$

where $\langle F \rangle$ is the expected value of the functional equation $F(x_1, x_2)$ with respect to the PDF $g(x_1, x_2)$. One can think of $g(x_1, x_2)$ as being proportional to the joint probability that $X_1 = x_1$ and $X_2 = x_2$, where $g(x_1, x_2) dx_1 dx_2$ is the probability that $x_1 \leq X_1 \leq x_1 + dx_1$ and $x_2 \leq X_2 \leq x_2 + dx_2$ (ref. 2). The representation of this multidimensional integral in two independent variables can be generalized to any number of independent variables.

According to the Monte Carlo method (ref. 2), an approximation to the integrand in equation (9) can be obtained by sum as follows:

$$\hat{F}(N) = \frac{1}{N} \sum_{j=1}^N F(x_{1j}, x_{2j}) \quad (10)$$

where $\hat{F}(N)$ is called the sample average and a number N of sample values (x_{1j}, x_{2j}) are picked from the PDF $g(x_1, x_2)^+$, where $g(x_1, x_2)^+$ is contained $g(x_1, x_2)$ and the function $F(x_1, x_2)$ is evaluated for each (x_1, x_2) (ref. 1). Here as in the Conroy method, $F(x_1, x_2)$ may be regarded as a periodic function. Thus, as is evident, both the Conroy and Monte Carlo methods for approximating the expected value $\langle F \rangle$ of the integrand are obtained by an averaging summation process in a similar manner.

The Monte Carlo method does not enable one to obtain accurate numerical values of the variables that appear in the integrand. These approximate numerical values do not necessarily bias the estimating procedure, rather

it only increases the statistical error of the calculation as compared with what would have been obtained had correct values been used. In other words, the Monte Carlo method is suggestive and normative rather than explicitly directive.

ERROR ANALYSIS FOR CONROY AND MONTE CARLO METHODS

There are two basic types of error one has to contend with in multi-dimensional integration. The first type results from the inaccuracy of the numerical values of the variables of the integrand. Since these values are the result of stochastic processes, one may calculate the error bound of the integrand by using an advance estimation technique called upper and lower limits of error. The second type of error results from the actual sampling process, whether it is done systematically or randomly. However, it is in the random sampling process that the greatest amount of statistical error occurs. Therefore, in the Monte Carlo method there are several reduction techniques used to reduce statistical sampling error (ref. 3) whereas in the Conroy method the systematic selection process guarantees the least amount of statistical error.

The upper and lower bound estimate technique is designed to estimate the magnitude of error to be anticipated in both the Conroy and Monte Carlo methods for periodic functions. In the Conroy integration scheme, the greatest concern is the method's capability of estimating the rate of improvement in accuracy as the number M of sample points is increased. As mentioned earlier, the P 's are the selected odd integers. It should be kept in mind that in estimating the maximum error anticipated for a given periodic function to be integrated, a new, appropriately constructed, set of integers, P , will be furnished for each new, larger value of M to be used. (See Table 1.)

Suppose that $F(\vec{x})$, where \vec{x} is k component vector, is to be integrated and that it represents an absolutely convergent Fourier series defined accordingly:

$$F(\vec{x}) = \sum_{\vec{n}} a_{\vec{n}} e^{i(\vec{n}, \vec{x})} \quad (11)$$

where $i = \sqrt{-1}$ and \vec{n} stands for the combination of integers $(n_1, n_2 \dots n_k)$, the summation $\sum_{\vec{n}}$ is multiple over the k dimensions with each index n_i in the range $(-\infty, \infty)$. Furthermore, suppose it is also the case that for every s such that $s > 0$ there exist a constant C_s , such that if none of the $n_i = 0$, we have (ref. 4):

$$|a_n| \leq C_s |n_1 n_2 \dots n_k|^{-s} \quad (12)$$

We will assume that, if any of the $n_i = 0$, the same inequality holds with the zero factors omitted from the denominator on the right-hand side.

Let the range of summation of the indices n_1, n_2, \dots, n_k be subdivided into V zones such that $N_i < n_i < 2N_i$, then given a fixed set P whose maximum positive value is denoted by $n \cdot P$ for a particular zone V may then be specifically designated as $(n \cdot P)_{\min}$. Therefore, for the zone V the range of possible values of the function $n \cdot P$ has the width W_V , i.e.,

$$W_V = (n \cdot P)_{\max} - (n \cdot P)_{\min} \quad (13)$$

The total number of combinations (n_1, n_2, \dots, n_k) that can occur within zone V is $|N_1, N_2, \dots, N_k|$. Only certain discrete values are solution eigenvectors of the Diophantine equation $n \cdot P = JM$ where J is an integer and M and P are fixed quantities. We must always construct our P 's so that neither M nor zero will ever be a submultiple of P_i , or of any simple sum or difference of the P_i because these eigenvectors will not contribute to the error eigenvectors, i.e., $|N_i| < 2$ (ref. 4). The number of eigenvectors generated by a zone V is approximately $P_V = |N_1 N_2 \dots N_k| M^{-1}$. However, for well-constructed sets P , the number may be less than P_V (ref. 3). None of the P_V eigenvector solutions to the Diophantine equation (see Appendix A) from zone V have a Fourier coefficient of magnitude $|a_n|$ larger than $C_s |N_1 N_2 \dots N_k|^{-s}$. Thus, the error bound can be written ascendingly as a summation over all zones, provided of course this summation converges (ref. 1).

The method for estimating error in the Monte Carlo method is the same as that used in the Conroy method for periodic functions. Any statistical estimate has an error which can be estimated in terms of the variance. In multidimensional integration, one may mathematically describe the variance accordingly, in general:

$$\begin{aligned} V &= \overline{[F(x_1, x_2) - \bar{F}]^2} \\ &= \frac{1}{N} \iint [F(x_1, x_2) - \bar{F}]^2 g(x_1 x_2) dx_1 dx_2 \\ &= \frac{1}{N} [\overline{F^2} - \bar{F}^2] \end{aligned} \quad (14)$$

Often it is profitable to change or at least distort the original problem in such a way so that uncertainty, due to random sampling in the solution, is reduced. Such procedures are known as variance reduction techniques, because uncertainty can be measured in terms of variance when the random sampling method is the basis of the multidimensional integration process.

There are six techniques of variance reduction that are most useful in estimating error in Monte Carlo calculations (ref. 2). They are: (1) Importance Sampling; (2) Russian Roulette and Splitting; (3) Use of Expected Values (combination of analytic and probabilistic methods); (4) Correlation and Regression; (5) Systematic Sampling; and (6) Stratified Sampling (Quota Sampling) (ref. 5).

In order to illustrate the general nature of the techniques, they are first applied to a very simple example and their brief discussion is included in Appendix B. The discussion of how the six techniques can be applied to the Monte Carlo evaluation of definite integrals is left for a subsequent publication. The integral is used as an example not because it is the main application of the technique - it is not (except in the generalized sense that any expected value can be calculated by an integral) - but rather because it is the application in which the ideas are most clearly explicated (ref. 5).

The simple example used in the problem of calculating the probability of obtaining a total of three when one tosses two ordinary dice. Each die is of the standard sort with six faces labeled from one to six and constructed so that each face has the probability (1/6) of being on top.

The problem can, of course, be solved analytically. Any particular combination of the dice has a probability equal to 1/6 times 1/6 of occurring. Since there are two combinations which make three (one-two and two-one), the probability of getting a three in a random toss of the dice is 2/36 or 1/18.

In doing the above problem by Monte Carlo, one would simply toss the dice N times, count the number (n) of successes (three's) and then estimate the probability (p) of success by

$$\hat{p} = \frac{n}{N} \quad (15)$$

Typically, \hat{p} differs from p ; that is, the estimate has a statistical error. This statistical error is usually measured by the standard deviation σ , where

$$\sigma = \frac{p(1-p)}{N} \quad (16)$$

The percent error E is then given by

$$E = \frac{100\sigma}{p} = 100 \frac{1-p}{N} \quad (17)$$

This implies that the error decreases as the number of trials is increased. However, as mentioned earlier, there are other ways, namely, the variance reduction techniques (Appendix B) by which the errors can be decreased.

MULTIDIMENSIONAL INTEGRATION WITH TWO INDEPENDENT VARIABLES

As an example of the multidimensional integration in two independent variables, the following simple double integral

$$I \int_0^{\pi/2} \int_0^{\pi/2} \cos^2 \theta_1 \cos^2 \theta_2 d\theta_1 d\theta_2 \quad (18)$$

is considered. Its exact analytical solution is

$$I = \frac{\pi^2}{16} = 0.61685$$

Against this exact result for equation (18), the results obtained by numerical integration by the Conroy and Monte Carlo methods are compared. In the Conroy method, the number of sample points, M , selected were 538 and 1154 for $k = 2$, the dimensions of the integration, as given in Table 1.

The sample point distribution was then generated by the values of (P_1, P_2) given for $M = 538$ and 1154 by using equation (3). The result is given by the summation in equation (2) in which e_1 and e_2 are equal to $\frac{1}{2}$ and $M = N/2$.

The results of the two-dimensional integration of equation (18) by the Conroy method, as well as the Monte Carlo method, are given in Table 2. They clearly show the greater accuracy and efficiency of the Conroy method over the Monte Carlo method and are discussed in the concluding section.

DOUBLE SCATTERING CONTRIBUTIONS TO SOLAR

AUREOLE RADIANCE

The approach adopted and the concepts and assumptions used in obtaining the expressions for the sky radiance due to the second and higher order of scattering have been explained in references 10, 11, and 12. Some of the salient features of the treatment are recapitulated as follows.

The basis of the theoretical treatment is (1) to treat the radiance due to multiple scattering as the sum of contributions due to the various orders of scattering, and (2) to consider the Nth order scattering as the result of N single scatterings.

The following reasonable simplifying assumptions have been made:

1. The atmosphere is treated as plane-parallel.
2. The atmosphere is composed of air molecules and (various species of) aerosols.
3. The atmosphere is vertically homogeneous in the size distribution and inhomogeneous in number density; i.e., the altitude size distribution is a separable function of the form

$$n(r,y) = n(r)\rho_A(y), \quad [\text{cm}^{-3}\mu\text{m}^{-1}] \quad (20)$$

which represents the case when the size distribution, $n(r)$, of the aerosols does not vary with altitude. $\rho_A(y)$ is a dimensionless parameter representing the altitude dependence of the total concentration (density) of the aerosol particles.

4. The atmosphere is horizontally homogeneous.
5. The effects of absorption, polarization, and ground reflection are ignored.

The geometry of the problem is illustrated in figure 1. The volume element, dV_1 , which in the case of single scattering (SS) is illuminated by light scattered by another volume, dV_2 , anywhere else in the surrounding space. The dihedral angle between the detector-zenith and zenith dV_2 planes is ω_1 , and that between dV_1 -zenith and zenith-sun planes is ω_2 . These are related to the dihedral angle ω_{ps} between the detector-zenith and the zenith-sun planes by the relation

$$\omega_2 = \pi + \omega_{ps} - \omega_1 \quad (21)$$

The first scattering takes place at dV_2 and the second at dV_1 (fig. 1):

$$dV_2 = R_2^2 \sin \phi_2 d\phi_2 d\omega_2 dy_2 \sec \phi_2 \quad (22a)$$

and

$$dV_1 = R_1^2 dR_1 d\Omega_1 = R_1^2 \sin \phi_p d\phi_p d\omega_1 dy_1 \sec \phi_p \quad (22b)$$

The scattering angles ψ_2 and ψ_1 , at the volumes dV_2 and dV_1 , respectively, are related to the directional angles as:

$$\cos \psi_2 = \cos \phi_s \cos \phi_2 - \sin \phi_s \sin \phi_2 \cos \omega_2 \quad (23a)$$

and

$$\cos \psi_1 = \cos \phi_p \cos \phi_2 - \sin \phi_p \sin \phi_2 \cos \omega_1 \quad (23b)$$

The altitude dependent volume scattering functions (VSF) F' are given by

$$F'(\psi_2, y_2) = \sum_i F_i(\psi_2) \rho_i(y_2) \quad [\text{km}^{-1} \text{sr}^{-1}] \quad (24a)$$

and

$$F'(\psi_1, y_1) = \sum_j F_j(\psi_1) \rho_j(y_1) \quad [\text{km}^{-1} \text{sr}^{-1}] \quad (24b)$$

where $i, j = M$ and A , represent the molecular (M) and aerosol (A) species that significantly contribute to the sky radiance, and F 's represent the VSF's.

The optical depths are determined for each path length just as in the SS analysis (ref. 8) and are defined by

$$\tau(y) = k(\lambda) \int_y^{\infty} \rho(y) dy \quad (25)$$

By tedious but straightforward mathematical manipulation, we may express the sky radiance due to dS in the form

$$B_2(\lambda, \phi_s, \omega_{ps}, \phi_p) = H_0(\lambda) \sec \phi_1 e^{-\tau(0) \sec \phi_1} I \quad (26)$$

where

$$I = \int_0^{\pi} dy_1 \int_0^{\pi} dy_2 \int_0^{\pi} \int_0^{2\pi} [\exp -\tau_a(y_1) D_{1a} + \tau_p(y_1) D_{1p}] \{F(\omega_2, \phi_2)\} \sec \phi_2 \sin \phi_2 d\omega_2 d\phi_2 \quad (27)$$

and

$$F(\omega_2, \phi_2) = F'(\psi_2, y_2) F'(\psi_1, y_1) e^{[\tau_a(y_1) - \tau_a(y_2)] D_{2a} + [\tau_p(y_1) - \tau_p(y_2)] D_{2p}} \quad (28)$$

$$D_{1a} = D_{1p} = -\sec \phi_p + \sec \phi_s, \quad D_{2a} = D_{2p} = \sec \phi_2' - \sec \phi_s \quad (29)$$

The following simple two-dimensional integral is considered for evaluation by the Conroy and Monte Carlo methods:

$$I_2 = \int_0^{\pi} \int_0^{\pi} F(\phi_2, \omega_2) f(\phi_2) d\omega_2 d\phi_2 \quad (30)$$

where

$$f(\phi_2) = \sec \phi_2 \sin \phi_2 \quad (31)$$

Transforming the variables of the definite integral so that the limits of integration are (0,1), one has

$$I_2 = 2\pi^2 \int_0^1 \int_0^1 F(\pi\omega_2, 2\pi\omega_2) f(\pi\phi_2) d\phi_2 d\omega_2 \quad (32)$$

Let $F_2(\pi\phi_2, 2\pi\omega_2) = F(\pi\phi_2, 2\pi\omega_2) f(\pi\phi_2)$, then one has

$$I_2 = 2\pi^2 \int_0^1 \int_0^1 F_2(\pi\phi_2, 2\pi\omega_2) d\omega_2 d\phi_2 \quad (33)$$

where ω_2 and ϕ_2 are independent variables,

a. Evaluation of equation (33) by the Conroy method:

The double scattering contributions to sky radiance were computed at four angular distances from the center of the sun at solar zenith angle $\phi_s = 57^\circ$, in the sun vertical, which is the plane passing through the detector, the sun and center of the earth. The zenith angles for the four angular directions were $\phi_p = 60^\circ, 63^\circ, 66^\circ$, and 72° . The double integral over the angular coordinates was evaluated by the Conroy method with both $M = 538$ and 1154. The results are shown in Table 3.

b. Evaluation of equation (33) by the Monte Carlo method:

For a description of the Monte Carlo procedure one is referred to several excellent papers on the subject (refs. 2-9). Since the main thrust of this paper was to compare the Conroy method with the Monte Carlo method in the solution of radiative transfer problems involving, for simplicity, only second order scattering, one restricts the computations to the same double integration over the two angular coordinates (ϕ, ω) as in the Conroy method, and to the same number of trial histories as the number of sample points in the Conroy scheme, namely, 538 and 1154. The results are shown in Table 3. In the Monte Carlo scheme, the azimuthal angle ω , and the zenith angle are given by $\omega = \pi(2R_1 - 1)$, and $\phi = \sin^{-1}(2R_2 - 1)$, where R_1 and R_2 represent random numbers.

DISCUSSION OF RESULTS AND CONCLUDING REMARKS

The aim of the paper was to discuss the basic features and the error analysis of the Conroy method for solving multidimensional integrals as applied to the problem of radiative transfer in a scattering atmosphere and, at the same time, compare these aspects with those of the Monte Carlo method. This being a preliminary study in the application of the Conroy

method to radiative transfer problems, the discussion is confined to simple examples of a physical and nonphysical process. The two methods were applied first to the multidimensional integration in two independent variables (θ_1, θ_2) of a trigonometric function $\cos^2 \theta_1 \cos^2 \theta_2$, and then, to simple problem of computing the second order light scattering contributions to the sky radiance. The former represents a typical nonphysical process and the latter, a typical physical process (ref. 9). The results of the numerical computations made by the two methods are shown in Tables 2 and 3. It is seen that the Conroy method gave results that agreed with exact analytic results for the trigonometric integrand to within 0.5 percent. On the other hand, the Monte Carlo method, for the same number of trial histories as the number of sample points in the Conroy method, produced results which agreed with exact values to within 2 percent. The agreement improved to within 1 percent as the number of trial histories was increased up to 5,000. This clearly shows the greater efficiency and accuracy of the Conroy method over the Monte Carlo method for the case of double integration of a mathematical function. On the other hand the results obtained for the second order scattering problem by the Monte Carlo method differed considerably from those obtained by the Conroy method. It seems that more trial histories for photons should be undertaken to reduce the discrepancy, thereby making it computationally far more expensive than the Conroy method. Of course, one realizes that to succinctly illustrate the greater efficiency of the Conroy method, the ideal procedure would have been to keep on increasing the number of trial histories in the Monte Carlo method till the results agree with those obtained by the Conroy method. However, because of constraints on computation costs, the present computational procedure was adopted, keeping in mind that the main thrust of the paper was to point out to the radiative transfer community the existence and the advantages of the Conroy method. Further work is planned to carry out the former procedure.

In the evaluation of the second order scattering problem, it is suggested that the three-dimensional integration over the angular and altitude position variables ϕ , ω and y , should be performed by both the Conroy and Monte Carlo methods. In remote sensing problems, often the numerical computations for solving the radiative transfer equation(s) become prohibitively expensive, and, therefore, it is essential that efficient methods be sought that increase the efficiency and reduce the computation costs. This paper has shown that the Conroy method is an efficient and economical method. It is, therefore, recommended that the use of the Conroy method be further explored in radiative transfer problems and particularly in solving cases which involve orders of scattering higher than two.

APPENDIX A

DIOPHANTINE EQUATIONS

Diophantine Equations is the name given a branch of mathematics on the theory of numbers. It treats the problem of finding the solutions, in integers of rational or complex (continued) fractions, for one or more conditional algebraic equations whose coefficients are rational. Fermat's Last Theorem on the integers, expressed by the generalized equation $x^n + y^n = z^n$, where x , y , and z represent the sides of a triangle, respectively, that are integral and n is an integer, is often referred to as a basic Diophantine Equation. From this generalized equation, one is able to show that $x = 2kmn$, $y = k(m^2 - n^2)$ and $z = k(m^2 + n^2)$, where k is an arbitrary positive integer, are all of the positive integral solutions of $x^n + y^n = z^n$. Another equation that is a topic of Diophantine analysis is the theory of quadratic forms, which is expressed in equation form as $ax^2 + bxy + cy^2 = m$, where x and y for a , b , and c are given integers. This equation may be solved by use of a linear transformation or by an older method known as continued fractions.

APPENDIX B

VARIANCE REDUCTION TECHNIQUES

1. Importance Sampling

If by some method one can increase the effective value of p , equation (17) shows that the percent error will be reduced. This increase in the effective value of p can be obtained very easily. One could, for example, bias the dice so that the probability that a one or a two would come up is twice as great as usual, that is $1/3$ rather than $1/6$. This could be done with physical dice by "loading" them, or with mathematically simulated dice by using a biased table of random numbers. If this is done, then the probability of getting a three, instead of being $1/18$, is four times as great or $2/9$. The percent error is then cut by slightly more than a factor of two. Of course, equation (15) can no longer be used to estimate p , but

$$\hat{p} = \frac{1}{4} \frac{n}{N} \quad (34)$$

must be used instead. The $1/4$ in equation (34) is called a weighting factor. By using it, the distortion introduced by the bias sampling is removed.

This illustrates the general idea of importance sampling - which is to draw samples from a distribution other than the one suggested by the problem and then to carry along an appropriate weighting factor which, when multiplied into the final results, corrects for having used the wrong distribution. The biasing is done in such a way that the probability of the sample's being drawn from an "interesting" region (ref. 3) is increased; the probability that it comes from an "uninteresting" region is correspondingly decreased. It seems correct to carry the bias to the limit; that is, the probability of getting a one or a two could be increased by a factor of three, making the probability of obtaining one of these numbers $1/2$ and making the probability of obtaining any other number zero.

The above limit is not the ultimate limit. For example, if one tossed the dice one at a time, then one might want to bias the second die differently from the first one. In particular, if one is willing to let the biasing of the second die depend on the outcome of the first throw, one might consider the following scheme.

1. Increase the probability of getting a one or a two on the first die by a factor of three. This means, of course, that there will be a zero possibility of getting any other numbers.

2. If the first die comes up one, increase the probability of the second die coming up two by a factor of six; if the first die comes up two, increase the probability of the second die coming up one by a factor of 6.

If this scheme is followed every toss of the dice will yield a three so that the number of successes (n) will be equal to the number of trials (N). The weighting factor will be $1/3$ times $1/6$ or $1/18$ and the estimate will be

$$\hat{p} = \frac{n}{18N} = \frac{1}{18} \quad (35)$$

which is exactly equal to p . We have devised a sampling procedure which has zero variance. In principle, though not in practice, it is always possible to design an importance sampling scheme that has zero variance.

2. Russian Roulette and Splitting (Ref. 3)

Let us assume that the dice are tossed one at a time and that the cost of the problem is measured by the total number of tosses. Now, it is immediately clear that if the first die is tossed and if it happens to come up three or greater, it will be impossible to get a total of three, no matter how the second die comes up. Under these circumstances, there is no point in making the second toss and we can simply record a zero for the experiment. This makes it unnecessary to toss the second die $2/3$ of the time. Therefore, on the average we will do $1/3$ fewer tosses in an experiment.

Generally, in more complicated examples where the sampling is done in stages, it is often possible to examine the sample at each stage and classify it as being in some sense "interesting" or "uninteresting." The sensible calculator is willing to spend more than an average amount of work on the "interesting" ones and contrarywise wants to spend less effort on the "uninteresting" ones. This can be done by splitting the "interesting" samples into independent branches, thus getting more of them, and by killing off some percent (in the above example 100 percent) of the "uninteresting" ones. The first process is splitting and the second Russian roulette.

The "killing off" is done by a supplementary game of chance. If the supplementary game is lost the sample is killed; if it is won, the sample is counted with an extra weight to make up for the fact that some other samples have been killed. The game has a certain similarity to the Russian game of chance played with revolvers and foreheads - whence the name.

The idea of Russian roulette and splitting is similar to the sequential sampling schemes of quality control, though quite different in detail (ref. 6). It was first thought of in connection with particle diffusion problems. Particles which get into interesting regions are split into n independent subparticles, each with one n th of the weight of the original particle. Particles which get into uninteresting regions are, in effect amalgamated into a fewer number of heavier particles. In this way the calculator achieves its goal of allocating its effort sensibly.

3. Use of Expected Values

If the sampling is being done in two stages, then even if one is not clever enough to calculate the combinatories of the whole problem, one still might be clever enough to notice that there is no point in tossing the second die; that is, once the first die is tossed, it is trivially easy to calculate the probability when we want to obtain a total of three. For example, when the first die comes up one, the only way one can get the three total is for the second die to come up two. This event obviously has a probability of $1/6$. Similarly if the first die comes up two, the only way to get three is for the second die to be one. This event has a probability of $1/6$. Finally, all the other possibilities for the first die (three to six) have a zero probability of giving three.

If one records the probabilities rather than toss the second die, then it is a fact that the average of these probabilities is an estimate of p . This method of doing the problem simultaneously reduces the number of tosses we need by a factor of two and decreases the variance, so that the tosses we do make are more effective.

The illustration is not artificial. In many probabilistic problems, it turns out that much of the variance or fluctuation is introduced by a part of the probabilistic problem which can be calculated analytically; while the probabilistic part, which is hard to calculate analytically, in fact, may not introduce much fluctuation. In these cases the sensible calculator combines analytic and probabilistic methods - calculating analytically that which is easy and Monte Carloing that which is hard.

The three techniques discussed above can be extremely effective in realistic applications. In some applications it was found that each technique has, by itself, decreased the effective variance by factors of the order of 10^4 to 10^6 (ref. 7). In most cases this means changing the problem from one which cannot be done because it would be too expensive or lengthy to one which is easily done on modern computing machines or even by hand computers.

The three techniques which will now be discussed are, in general, not as effective as the three already mentioned. However, they often are very easy to use and may yield substantial improvements.

4. Correlation and Regression

In order to illustrate this technique, it will be necessary to change the example slightly. Assume, for instance, that the proprietor of a gaming establishment wishes to change the rules in force at his dice tables. Under the current rules, if a player tosses a 2, 3, or 12, on the first throw of the dice, the player loses. If he tosses a 7 or 11, he wins, and if he tosses a 4, 5, 6, 8, 9, or 10, he will win or lose, depending on whether or not the number or a 7 comes up first in his subsequent throws.

Now let the rule change being considered be the interchange of the roles of 3 and 4 and assume that, unlike most of the other proprietors, the one that is being considered is unsophisticated and wishes to determine by sampling what the change in his revenue will be. The obvious way to do this is to run two sets of experiments, one with the old rules and one with the new rules, and then compare the two experimentally-determined revenues. Under these circumstances, one is subtracting two relatively large, fluctuating quantities to determine a small quantity. In general, this yields a process with a large percent error.

There is a better way to do this problem. Instead of running two independent games, the proprietor could run only one game and apply both sets of rules simultaneously to this game. In fact, he can choose to estimate the difference in revenue directly rather than the revenue that would be achieved under each set of rules.

This can be done by playing the following game:

1. Whenever a 3 comes up, continue to toss the dice until either a 3 or 7 comes up. In the first happenstance, record a minus two, since under the old rules the customer would have lost a dollar, but under the new rules he wins one; in the second happenstance, record a zero because under both sets of rules the customer loses.
2. Follow a similar process if a 4 comes up.
3. If a number other than 3 or 4 comes up terminate the plan then and there and record a zero. (Because of this rule, the effects of chance fluctuations in the proportionate number of times that the numbers 2 and 5 to 12 come up are eliminated from the comparison.)

It should be noticed that the specific game that is played is quite different from the two games that are being compared. As usual, this causes a double saving of efficiency; first because only one set of games is played, and second because the number and kinds of chance fluctuations that can affect the results are greatly reduced.

It is, in fact, generally true that if we wish to compare two or more situations, we can, by combining this comparison into a single problem, reduce the work substantially. Only one problem, rather than several, has to be done, and the direct estimate of the difference can usually be made more accurately than estimates on separate individual quantities.

This is a substantial virtue of the Monte Carlo method. In many complicated problems one is not actually interested in absolute values but only in comparisons. One may wish, for example, to know if strategy A is better than strategy B, or if engineering design A is better than engineering design B. One might, in fact, not even believe the absolute values because the idealizations are so rough, but one does believe the qualitative features implied by differences. Monte Carlo can then be

used to estimate the thing which we actually desire to know and which one believes and one can bypass the estimate of irrelevant quantities. Usually, however, one can obtain these also, but at some extra cost.

Correlated sampling can also often be used to test the accuracy of an approximate theory (ref. 3). If the approximate theory happens to be an exact treatment of an idealized situation, and if the idealized situation happens to be "structurally" similar to the unidealized situation, then it is often possible to design very efficient sampling schemes to calculate the difference between the idealized and unidealized situations. The answer to the problem posed by the unidealized situation can then be obtained by adding together the results of the approximate analytic calculation and the Monte Carlo difference calculation.

5. Systematic Sampling

If one is doing a multistage sampling problem, it often turns out to be very easy to do the first stage systematically (ref. 7). For example, the problem under consideration, if one is going to toss the dice one at a time then there is really no point in actually tossing the first die. If, for example, one is planning on getting 600 samples, one would expect on the average that each die would come up one about 100 times, two another 100, and so on. It is easy to show that one does not bias the results if one assumes that the first 100 tosses of the first die actually do come up one, the second 100 tosses of this die come up two, etc., and so only toss the second die. The main advantage in doing this is that one has eliminated the error caused by the fluctuation in the proportions of ones, twos, etc., which would result if the first toss was random.

In practice, however, doing the first stage of the sampling systematically does not usually lead to substantial improvements in efficiency. Generally, in fact, it will only reduce the number of samples required by a relatively few percent - say 5 to 30. However, it ordinarily does not cost anything to apply this technique, so that there is no point in not using it. About the only time one may not be able to use it conveniently is when one does not know in advance how big a sample one will want.

6. Stratified Sampling

This last technique is a sort of combination of importance sampling and systematic sampling. For example, if one is only a little bit sophisticated and is doing the systematic sampling described above, one would soon notice that there is no point in considering the 400 tosses in which one had assigned the values three to six for the first toss of the die, since under these circumstances, one can never get a total of three. Therefore, we might systematically divide the sample into halves rather than sixths. In the first half we would say that the first die came up one, and in the second half that the first die came up two.

In theory, this method could be as powerful as importance sampling. In actual practice, the fact that you have to sample systematically turns out to decrease sharply the number of places in which it can be used. However, where it can be used, it is usually better than importance sampling and in any case never worse. Therefore, whenever the costs of the two techniques are comparable, stratified sampling is preferable to importance sampling (ref. 3).

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Table 1.- Optimized Parameters (M,P) for Multiple Quadratures by Conroy Method (Ref. 1)

k = 2						k = 3					
M	52	538	1154	3722	6044	M	52	538	1154	3722	6044
P ₁	15	171	177	1259	1427	P ₁	5	115	11	653	595
P ₂	25	177	415	1403	1891	P ₂	7	241	369	1005	1359
						P ₃	11	251	569	1483	1865
k = 4						k = 5					
M	1154	3722	6044			M	1154	3722	6044		
P ₁	103	119	687			P ₁	107	263	681		
P ₂	217	203	1385			P ₂	211	1049	1113		
P ₃	453	235	2843			P ₃	225	1145	1163		
P ₄	521	1849	2933			P ₄	459	1441	1853		
						P ₅	547	1759	2349		
k = 6						k = 7					
M	1154	2008	3722	6044	9644	M	1154	3722	6044		
P ₁	17	177	205	587	1177	P ₁	3	669	35		
P ₂	71	451	399	671	1269	P ₂	5	819	397		
P ₃	151	453	679	673	1625	P ₃	37	845	1427		
P ₄	203	565	1051	1459	1947	P ₄	377	857	1467		
P ₅	209	665	1163	2363	3369	P ₅	393	1379	1891		
P ₆	385	833	1811	2697	4087	P ₆	479	1421	2805		
						P ₇	559	1439	2865		
k = 8						k = 9					
M	3708	6044	9644			M	3722	6044	9644		
P ₁	151	43	129			P ₁	119	43	457		
P ₂	187	61	525			P ₂	339	87	509		
P ₃	333	179	2373			P ₃	437	179	1677		
P ₄	357	1421	2731			P ₄	773	1421	1723		
P ₅	839	1479	3351			P ₅	937	1479	2173		
P ₆	947	2039	4145			P ₆	1219	1589	2423		
P ₇	1245	2189	4119			P ₇	1503	2189	2489		
P ₈	1839	2783	4767			P ₈	1697	2191	3431		
						P ₉	1747	2783	3719		
k = 10						k = 11					
M	3722	6044	9644			M	3722	6044	9644		
P ₁	153	43	53			P ₁	39	159	205		
P ₂	223	87	263			P ₂	41	289	723		
P ₃	517	89	893			P ₃	51	309	731		
P ₄	859	179	1121			P ₄	481	349	1693		
P ₅	861	1421	1259			P ₅	649	471	2215		
P ₆	911	1479	2945			P ₆	671	523	2383		
P ₇	991	1589	3281			P ₇	705	727	2583		
P ₈	995	2095	4397			P ₈	1213	847	2787		
P ₉	1453	2191	4727			P ₉	1297	951	2961		
P ₁₀	1705	2783	4801			P ₁₀	1559	1665	3061		
						P ₁₁	1719	2899	3123		
k = 12						k = 13					
M	3722	6044	9644			M	3722	6044	9644		
P ₁	97	179	973			P ₁	97	179	973		
P ₂	419	795	1095			P ₂	419	795	1095		
P ₃	435	1073	1495			P ₃	435	1073	1495		
P ₄	477	1233	1853			P ₄	477	1233	1853		
P ₅	641	1359	2619			P ₅	641	1359	2619		
P ₆	717	1589	3365			P ₆	717	1589	3365		
P ₇	793	1667	3493			P ₇	793	1667	3493		
P ₈	1141	1675	3567			P ₈	1141	1675	3567		
P ₉	1163	1677	3595			P ₉	1163	1677	3595		
P ₁₀	1359	1917	3863			P ₁₀	1359	1917	3863		
P ₁₁	1535	2095	4063			P ₁₁	1535	2095	4063		
P ₁₂	1787	2189	4497			P ₁₂	1787	2189	4497		

Table 2.- Multidimensional Integration in Two Independent Variables

$$I = y_1 \int_0^{\pi/2} \int_0^{\pi/2} \cos^2 \theta_1 \cos^2 \theta_2 d\theta_1 d\theta_2$$

No. of Sample Points	CPU Time (Secs)	I	
		Conroy	Monte Carlo
538	0.151	0.61672	
	0.169		0.61667
1154	0.155	0.61672	
	0.178		0.61669

Table 3.- Second Order Scattering Contribution to Sky Radiance
(Double Integration over Angular Coordinates).

Solar Zenith Angle $\phi_s = 57^\circ$

No. of Sample Points/ Trial Histories	Observation Zenith Angle ϕ_p in Sun Vertical	Double Scattering Contribution I_2			
		Conroy		Monte Carlo	
		CPU Time (Secs)	I_2	CPU Time (Secs)	I_2
538	60°	62.6	.3675(-2) *	8.17	.1108(-2)
	63°		.3841(-2)		.5173(-2)
	66°		.4001(-2)		.4922(-2)
	72°		.4354(-2)		.3501(-2)
1154	60°	68.9	.3472(-2)	85.5	.1187(-2)
	63°		.3632(-2)		.1624(-2)
	66°		.3808(-2)		.8342(-2)
	72°		.4060(-2)		.5202(-2)

*The number within the parenthesis represents the power of 10, e.g.,
(-2) denotes 10^{-2} .

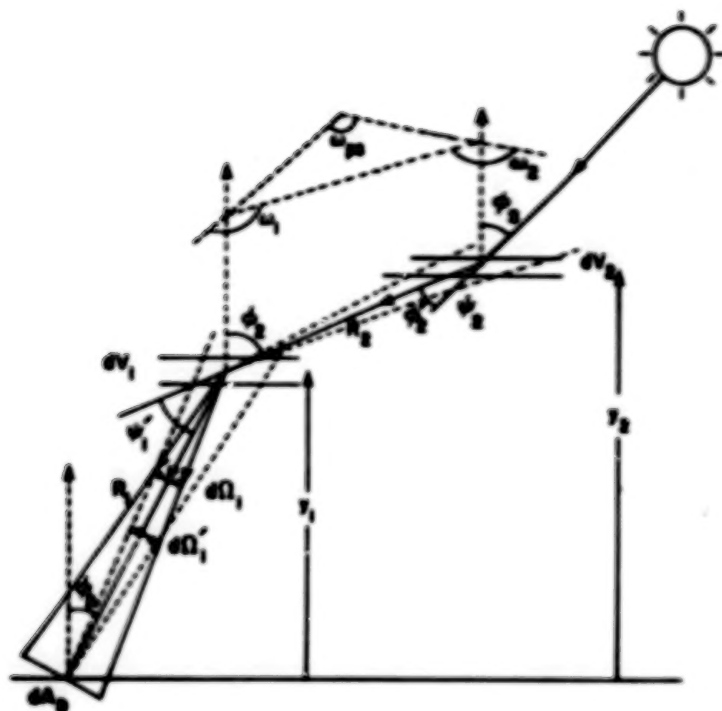


Figure 1.- Geometry illustrating the double scattering of sunlight by the atmosphere.

END

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